Sputtering of Materials for MEBT Absorber and PXIE Beam Dump

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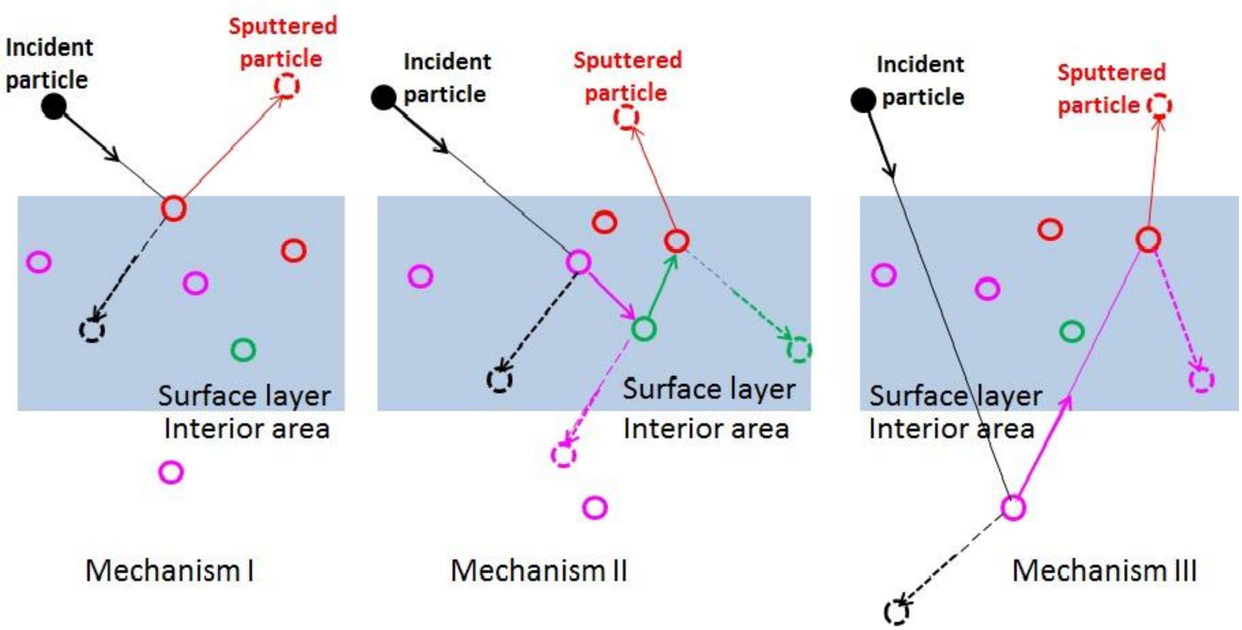
Abstract: Effect of sputtering was analyzed for different materials used for the MEBT absorber and beam dump of PXIE. The known experimental data are presented as well as the method of calculations, consistent with these data. Rate of yield of the sputtered atoms is estimated for nickel and molybdenum, used as materials for the MEBT absorber and PXIE beam dump, respectively. It is shown that the parameters of the proton beam in the fall it on molybdenum MEBT absorber (2.1 MeV x 10 mA = 21 kW) and on the nickel PXIE beam dump (30 MeV x 1.7 mA = 50 kW) the phenomenon of sputtering target material is negligible in terms of expected duration of operation of these devices.

Introduction

It is well known that puttering is a process whereby atoms are ejected from a solid target material due to bombardment of the target by energetic particles. The sputtering mechanism is caused by the following events [1-4]:

I. Direct knock-out collisions with incident ions at the solid surface;
II. Collision cascades created by incoming ions near the solid surface;
III. Collision cascades generated by ions backscattered from the interior of the solid.

All these mechanisms are presented schematically:



The following table shows what kind of mechanism is preferred for light / heavy ions in their normal, oblique and grazing incidence to the surface:

Table 1. Preferred mechanisms of sputtering for light/heavy ions.

Incidence	Normal	Oblique	Grazing
Light Ions	III	II and I	I and II
Heavy Ions	–	II and I	II and I

Further for materials of interest the experimental data will be presented, as well as the corresponding empirical formulas which allow evaluating the sputtering when the energies of incident particles are outside the measured values. Rates of yield of the sputtered atoms are estimated for nickel and molybdenum, used as material for the MEBT absorber and PXIE beam dump, respectively.

Normal incident

The following parameters and empirical formulas are used to describe the sputtering at normal incidence of particles of mass M_1, charge Z_1 and kinetic energy E on the surface of a material with M_2, Z_2 [5,6]:

- (1) Energy transfer factor $\gamma = \dfrac{4M_1M_2}{M_1+M_2}$;
- (2) Coefficient to factorize the cross section
$$\alpha^*(M_2/M_1) = \begin{cases} 0.249\cdot(M_2/M_1)^{0.56} + 0.0035\cdot(M_2/M_1)^{1.5}, & \text{for } M_1 \le M_2, \\ 0.0875\cdot(M_2/M_1)^{-0.15} + 0.165\cdot(M_2/M_1), & \text{for } M_1 \ge M_2 \end{cases};$$
- (3) Lindhart electronic stopping coefficient
$$k_e = 0.079\frac{(M_1+M_2)^{3/2}}{M_1^{3/2}M_2^{1/2}}\frac{Z_1^{2/3}Z_2^{1/2}}{(Z_1^{2/3}+Z_2^{2/3})^{3/4}};$$
- (4) Reduced energy
$$\varepsilon(E) = \frac{0.03255}{Z_1Z_2\sqrt{Z_1^{2/3}+Z_2^{2/3}}}\frac{M_2}{M_1+M_2}E;$$
- (5) Reduced nuclear stopping cross section (Tomas-Fermi model)
$$S_n^{TF}(\varepsilon) = \frac{3.441\sqrt{\varepsilon}\cdot\ln(\varepsilon+2.718)}{1+6.355\sqrt{\varepsilon}+\varepsilon(6.882\sqrt{\varepsilon}-1.708)};$$
- (6) Reduced nuclear stopping cross section
$$S_n(E) = 84.78\frac{Z_1Z_2}{\sqrt{Z_1^{2/3}+Z_2^{2/3}}}\frac{M_1}{M_1+M_2}S_n^{TF}(\varepsilon);$$

- (7) Values U_s, $Q(Z_2)$, $W(Z_2)$ and $s(Z_2)$ can be found from the following table using Z_2 for selected material:

target	Z_2	U_s	Q	W	s
Be	4	3.32	1.66	2.32	2.5
B	5	5.77	2.62	4.39	2.5
C	6	7.37	1.70	1.84	2.5
Al	13	3.39	1.0	2.17	2.5
Si	14	4.63	0.66	2.32	2.5
Ti	22	4.85	0.54	2.57	2.5
V	23	5.31	0.72	2.39	2.5
Cr	24	4.10	0.93	1.44	2.5
Mn	25	2.92	0.95	0.88	2.5
Fe	26	4.28	0.75	1.20	2.5
Co	27	4.39	1.02	1.54	2.5
Ni	28	4.44	0.94	1.33	2.5
Cu	29	3.49	1.0	0.73	2.5
Ge	32	3.85	0.59	2.08	2.5
Zr	40	6.25	0.54	2.50	2.8
Nb	41	7.57	0.93	2.65	2.8
Mo	42	6.82	0.85	2.39	2.8
Ru	44	6.74	1.31	2.36	2.5
Rh	45	5.75	1.14	2.59	2.5
Pd	46	3.89	0.85	1.36	2.5
Ag	47	2.95	1.08	1.03	2.8
Sn	50	3.14	0.47	0.88	2.5
Tb	65	4.05	0.90	1.42	2.5
Tm	69	2.42	0.65	0.85	2.5
Hf	72	6.44	0.65	2.25	2.5
Ta	73	8.1	0.56	2.84	2.8
W	74	8.9	0.72	2.14	2.8
Re	75	8.03	1.03	2.81	2.5
Os	76	8.17	1.11	2.86	2.5
Ir	77	6.94	0.96	2.43	2.5
Pt	78	5.84	1.03	3.21	2.5
Au	79	3.81	1.08	1.64	2.8
Th	90	6.2	0.63	2.79	2.5
U	92	5.55	0.66	2.78	2.5

- (8) Coefficient $\Gamma = \frac{1}{1+(M_1/7)^3} W$;
- (9) Sputtering threshold energy

$$E_{th} = U_s \cdot \begin{cases} 6.7\gamma^{-1} & \text{for } M_1 \geq M_2, \\ \frac{1+5.7\cdot(M_1/M_2)}{\gamma} & \text{for } M_1 \leq M_2 \ . \end{cases}$$

After that the yield sputtering is determined from the following expression:

$$Y(E) = 0.042 \frac{Q(Z_2)\cdot\alpha^*(M_2/M_1)}{U_s} \frac{S_n(E)}{1+\Gamma\cdot k_e\cdot\varepsilon(E)} \left[1-\sqrt{\frac{E_{th}}{E}}\right]^{s(E)} . \qquad (10)$$

The next piece is taken from [7].

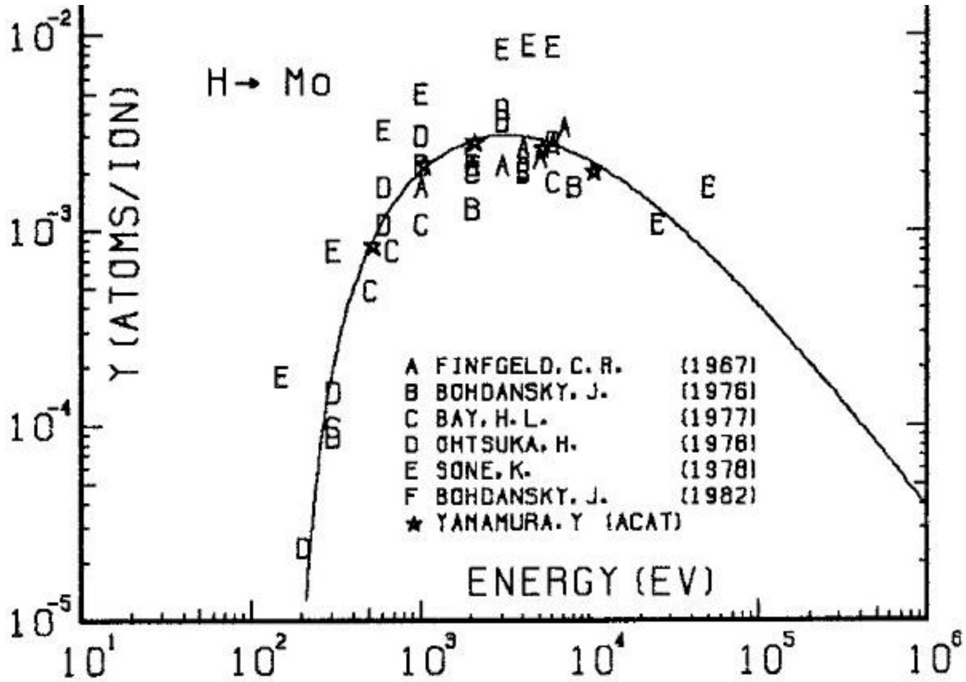
A few different computer codes are existed to simulate the sputtering process. Depending on how atomic collisions occur in a solid are modeled, these codes are basically classified into two groups: a) Monte Carlo (MC) codes which treat atomic collisions with MC method in a binary collision approximation (BCA); b) Classical molecular dynamics (MD) codes which assume that incident projectiles collide with a system of many atoms and solve time evolutionary the classic dynamics of the system from knowledge of the interaction forces between particles. Generally, MC codes are suitable for simulations in much larger space- and timescales than MD ones. However, as incident energy of ions reaches a low-energy range, e.g. around 100 eV, the effective iterative region that a moving atom feels widens. Accordingly, BCA breaks down, and MD is required, instead. Here is a brief description of existing codes.

The ACAT [8] and TRIM [9,10] are of the MC types. While the TRIM code pursues atomic collisions by using a mean free path similarly to many other MC codes, the ACAT code assumes an amorphous target by employing the so-called “cell model,” i.e. an amorphous target is composed of a simple cubic cells, in each of which the site of a target atom is chosen stochastically. “

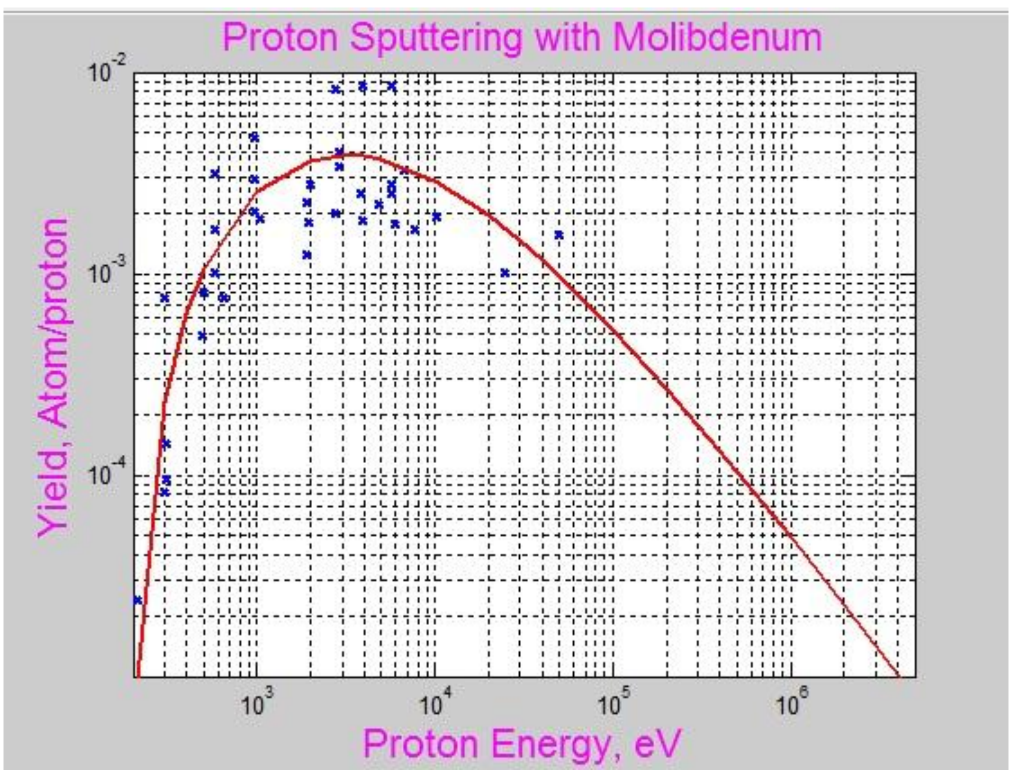
For more detailed description of the existing code with the corresponding references refer to [7].

Experimental data, simulations (code ACAT) and evaluations for some materials

<u>MOLIBDENUM</u>

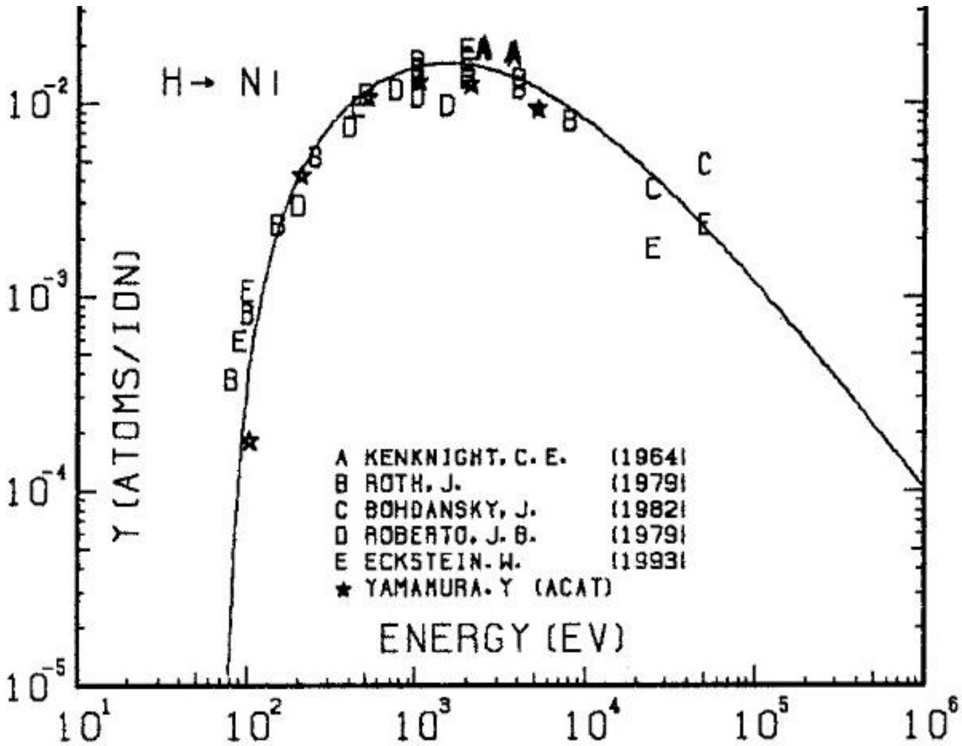


Experimental data and simulation from Fig. 164 [6].

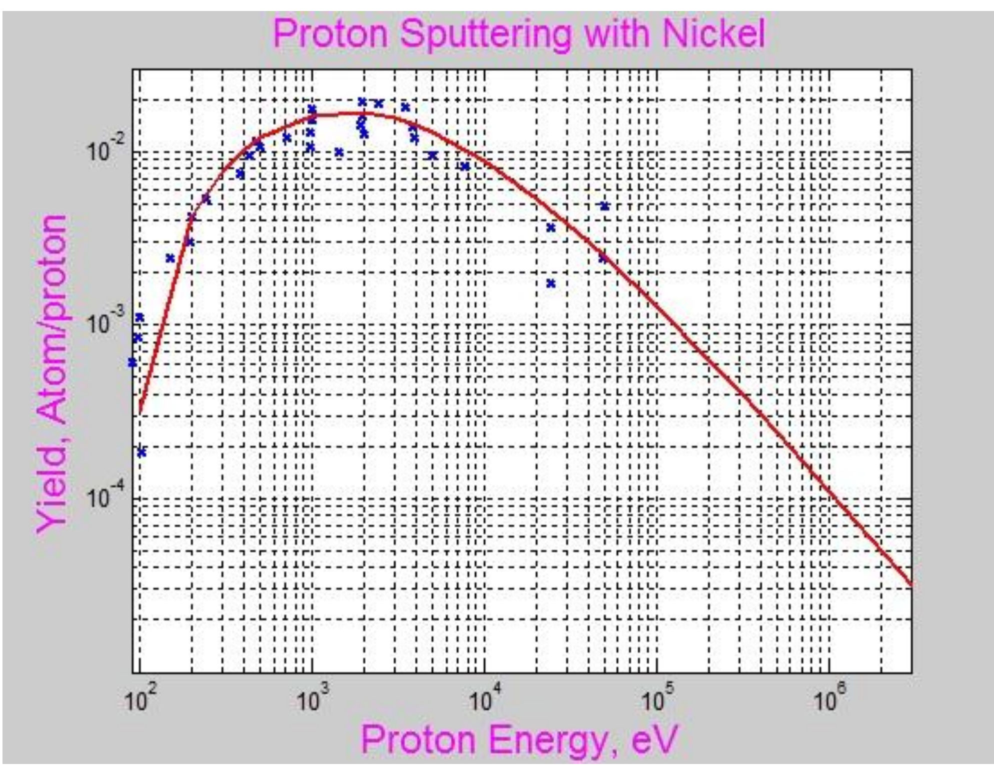


Experimental data from Fig. 164 [6], evaluation according to formulas (1) – (10).

NICKEL

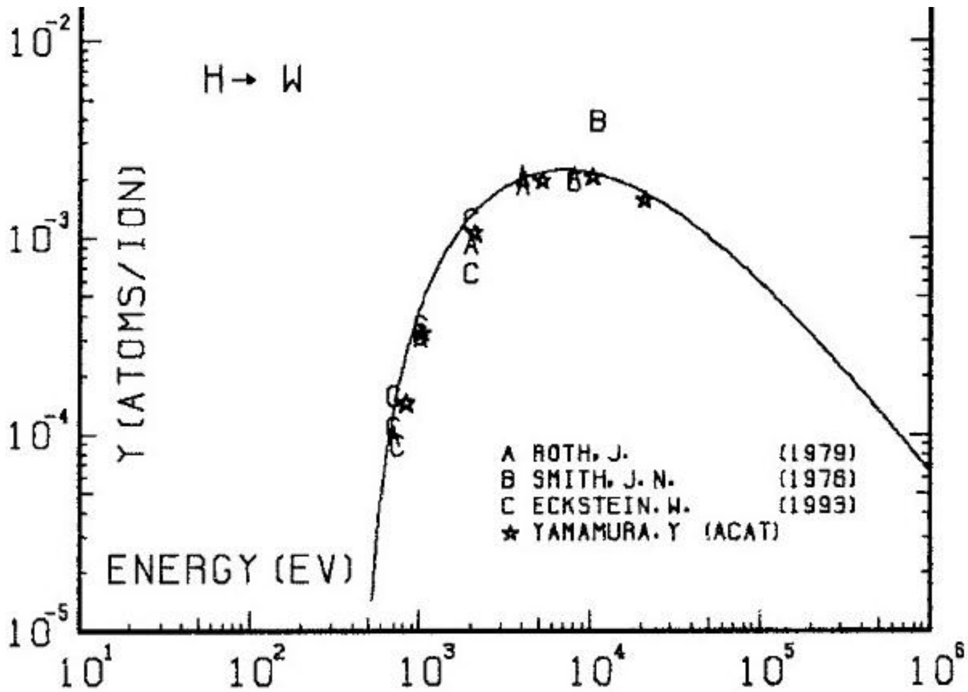


Experimental data and simulation from Fig. 99 [6].

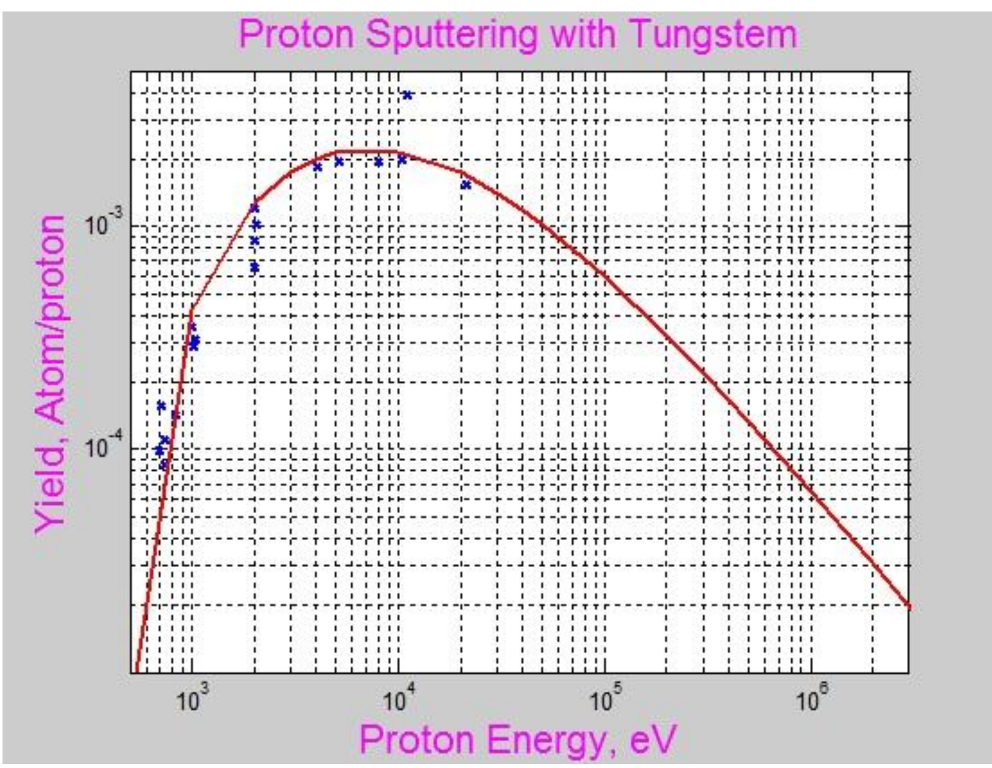


Experimental data from Fig. 99 [6], evaluation according to formulas (1) – (10).

TUNGSTEM

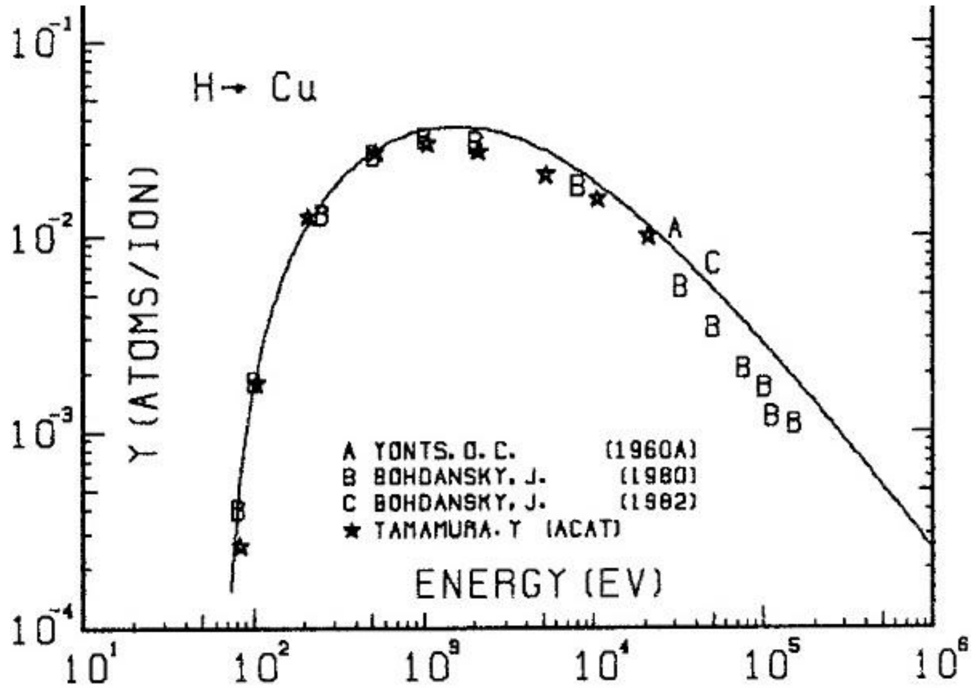


Experimental data and simulation from Fig. 255 [6].

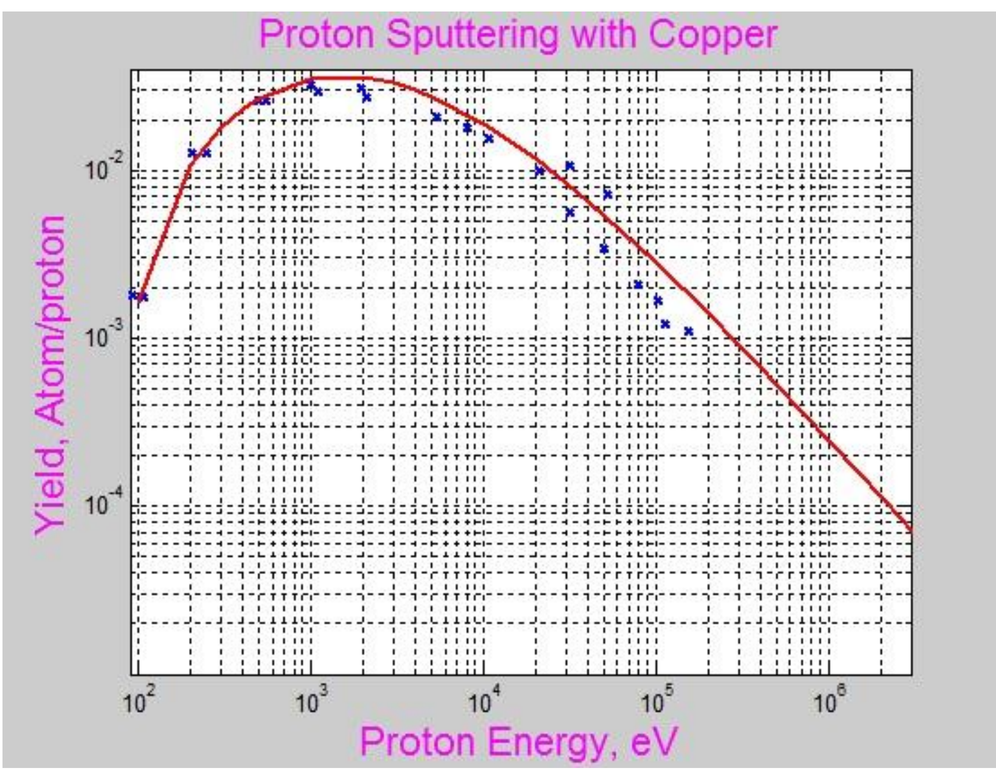


Experimental data from Fig. 255 [6], evaluation according to formulas (1) – (10).

COOPER

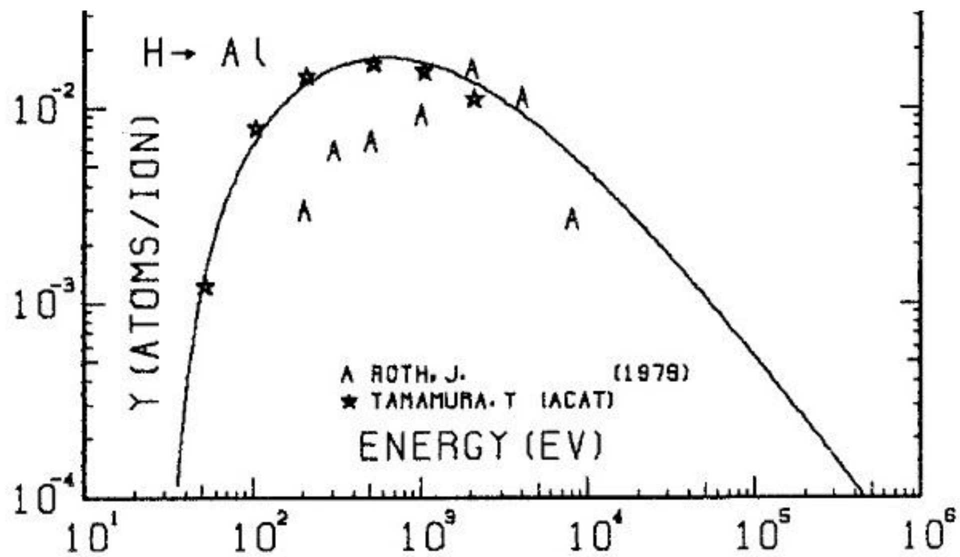


Experimental data and simulation from Fig. 110 [6].

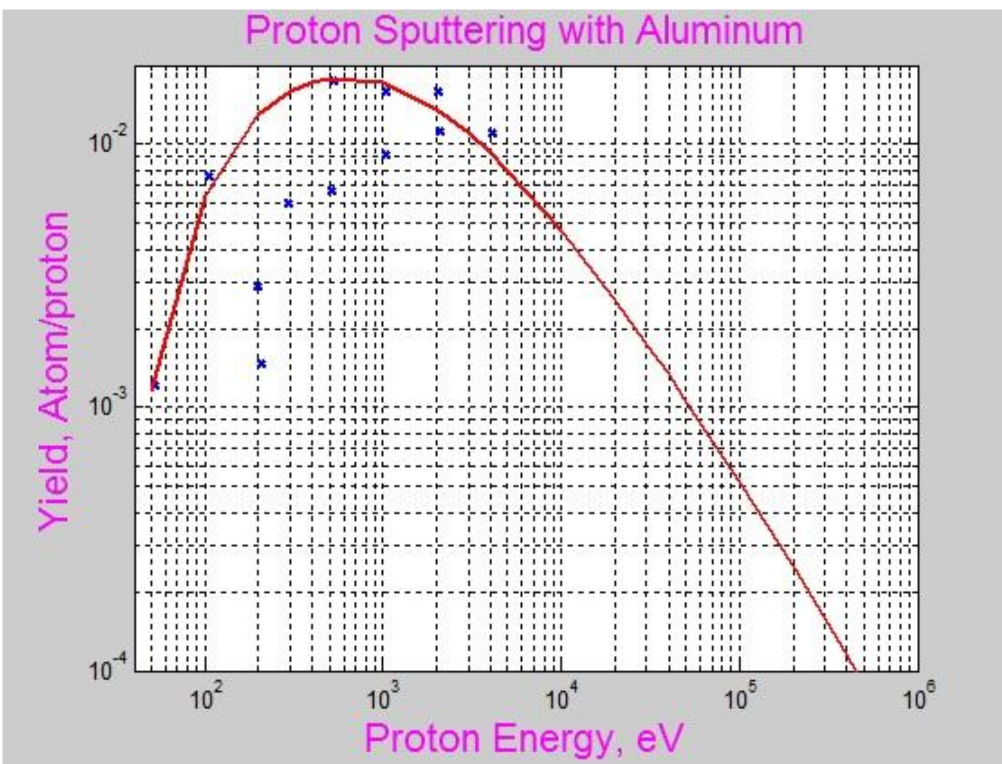


Experimental data from Fig. 110 [6], evaluation according to formulas (1) – (10).

ALUMINUM

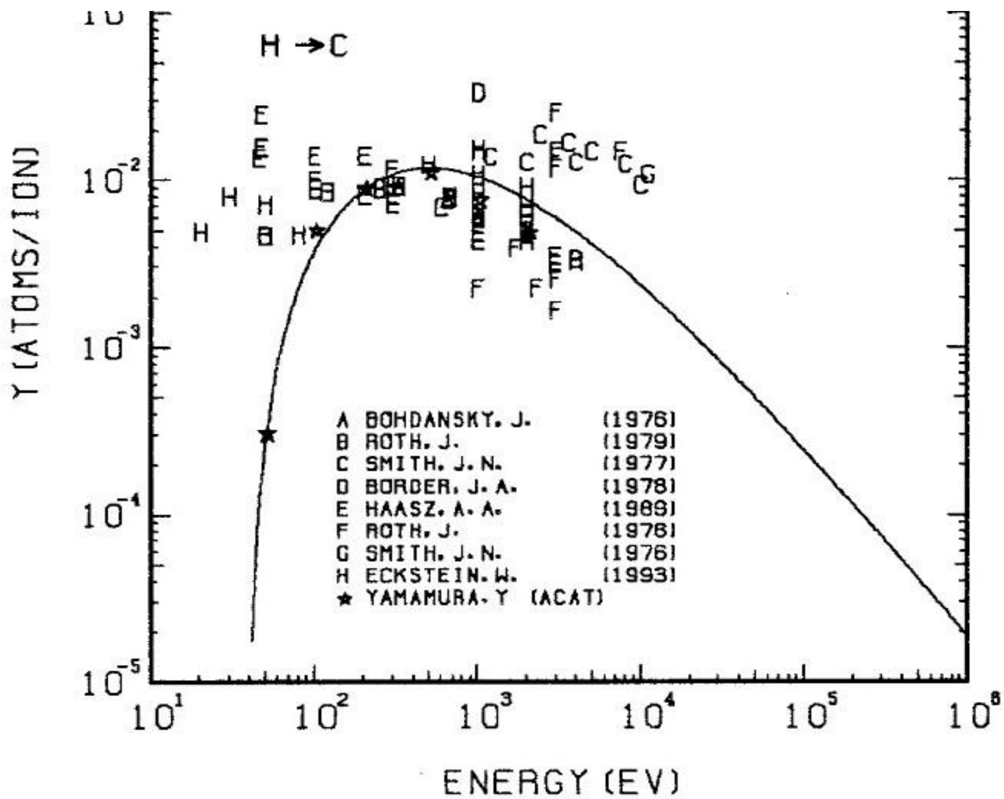


Experimental data and simulation from Fig. 26 [6].

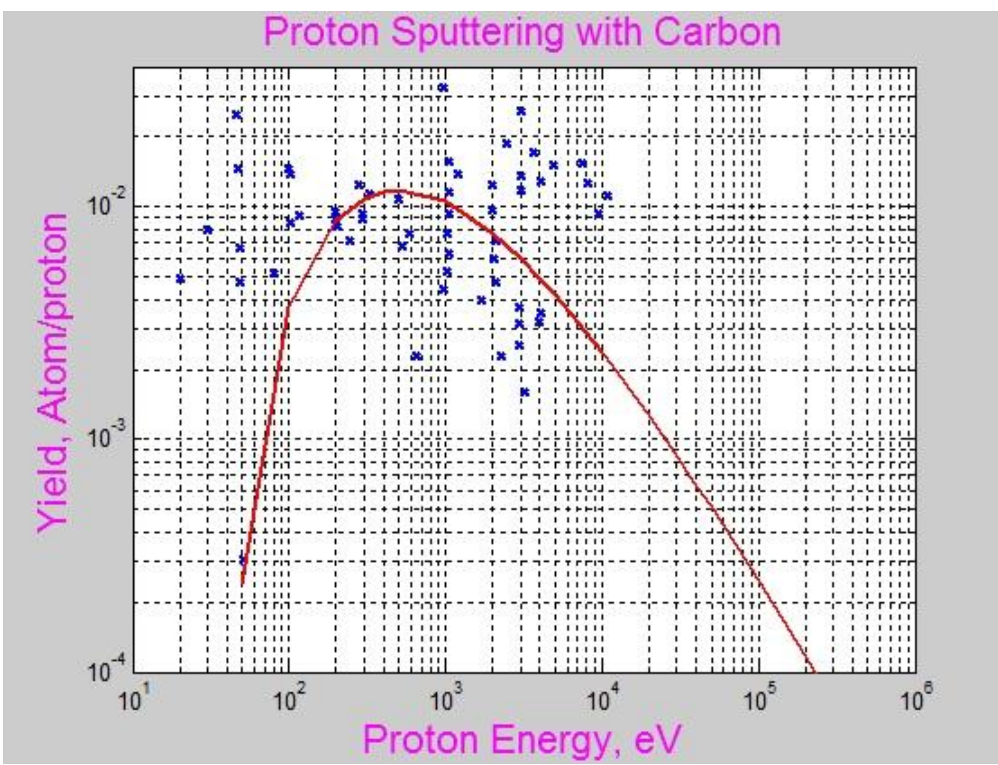


Experimental data from Fig. 26 [6], evaluation according to formulas (1) – (10).

CARBON

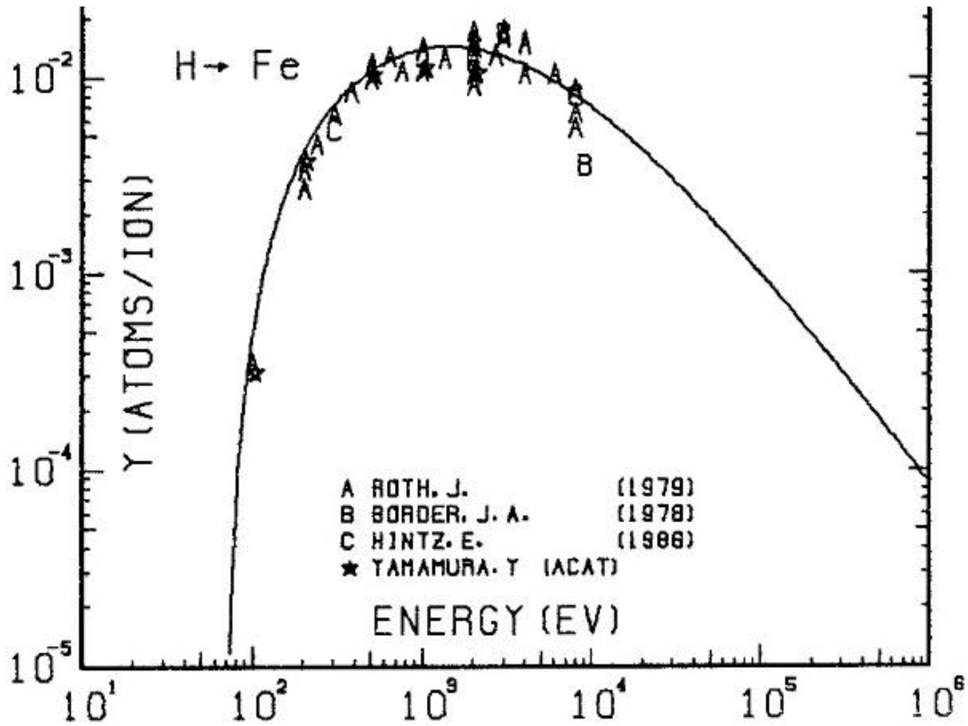


Experimental data and simulation from Fig. 15 [6].

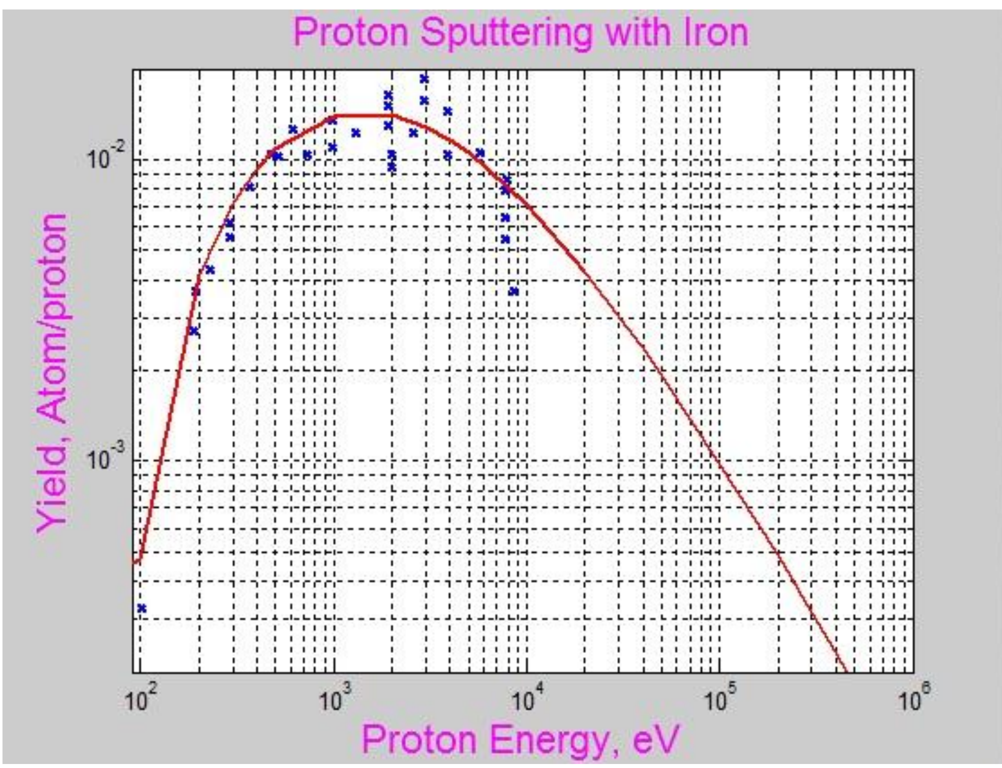


Experimental data from Fig. 15 [6], evaluation according to formulas (1) – (10).

IRON

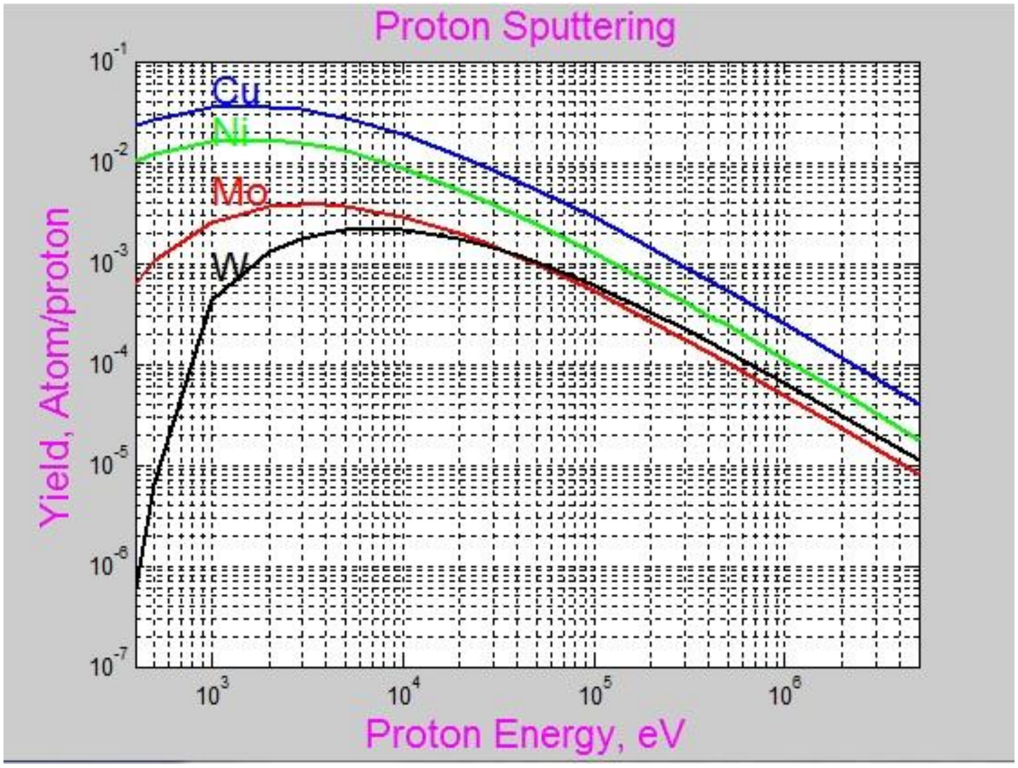


Experimental data and simulation from Fig. 78 [6].



Experimental data from Fig. 78 [6], evaluation according to formulas (1) – (10).

Yield Sputtering Evaluations for Some Materials of interest



These data show that nickel is more preferable in comparison with copper (the choice of material for PXIE beam dump), and for energy ~2.1 MeV (MEBT absorber) molybdenum and tungsten are practically identical to the yield of sputtering atoms.

MEBT Absorber: Sputtering for some materials

Input data to estimation:

Beam: $E_0 = 2.1\text{ MeV}; \quad I = 5\text{ mA} \rightarrow N_p \approx 3\cdot 10^{16}\text{proton/sec},$

$\sigma_x = \sigma_y = 2\text{ mm};$

Absorber: $\theta_{ab} = 29\text{ mrad}, \quad S_{ab} \approx \dfrac{2\pi\sigma_x\sigma_y}{\theta_{ab}} \approx 8.7\text{ cm}^2;$

Year: $T = 3600\cdot 24\cdot 365 \approx 3.15\cdot 10^7\text{ sec.}$

$$V_{atom} = \frac{m_{proton}\cdot M_{atom}}{d};$$

$$S_{[sec]} = Y\cdot N_p, \quad S_{[year]} = S_{[sec]}\cdot T;$$

$$S_{[mm]} = 10\cdot\frac{S_{[year]}\cdot V_{atom}}{S_{ab}}.$$

These input data are used to evaluate the yield for material of MEBT absorber in continuous operation for one year with 5 mA of proton beam with energy 2.1 MeV.

Value/Material	Molibdenum	Nickel	Copper	Tungstem
d, Density, g/cm^3	10.2	7.81	8.92	19.25
M_{atom}, Weigth of atom, aum	95.94	58.69	63.55	183.8
V_{atom}, Volume of atom, cm^3	$1.57\cdot10^{-23}$	$1.26\cdot10^{-23}$	$1.19\cdot10^{-23}$	$1.60\cdot10^{-23}$
Y, Yield, atom/proton	$2.1\cdot10^{-5}$	$4.8\cdot10^{-5}$	$1.1\cdot10^{-4}$	$2.9\cdot10^{-5}$
$S_{[sec]}$, Sputtering, atom/sec	$6.4\cdot10^{11}$	$1.4\cdot10^{12}$	$3.2\cdot10^{12}$	$8.7\cdot10^{11}$
$S_{[year]}$, Sputtering, atom/year	$2.0\cdot10^{19}$	$4.5\cdot10^{19}$	$1.0\cdot10^{20}$	$2.7\cdot10^{19}$
$S_{[mm]}$, Sputtering, mm/year	$3.7\cdot10^{-4}$	$6.6\cdot10^{-4}$	$1.4\cdot10^{-3}$	$5.1\cdot10^{-4}$
Maximal values (for corresponding proton energy, keV)				
Y, Yield, atom/proton	$3.9\cdot10^{-3}$(3.5)	$1.7\cdot10^{-2}$(≈ 2)	$3.6\cdot10^{-2}$(≈ 2)	$2.2\cdot10^{-3}$(0.8)
$S_{[sec]}$, Sputtering, atom/sec	$1.2\cdot10^{14}$	$5.0\cdot10^{14}$	$1.1\cdot10^{15}$	$6.5\cdot10^{13}$
$S_{[year]}$, Sputtering, atom/year	$3.6\cdot10^{21}$	$1.6\cdot10^{22}$	$3.4\cdot10^{22}$	$2.0\cdot10^{21}$
$S_{[mm]}$, Sputtering, mm/year	0.066	0.464	0.228	0.037

These data show that at the current of ~10 mA and continuous (during one year), bombarding of molybdenum absorber by 2.1 MeV protons due to sputtering it no more than 1 μm of material can be lost due to sputtering. Even at the energy corresponding to the maximum of sputtering yield (~3.5 keV), the loss will not exceed 0.1 mm per year.

PXIE beam dump: Sputtering for some materials

Input data to estimation:

Beam: $E_0 = 30$ MeV; $I = 1.7$ mA $\rightarrow N_p \approx 1\cdot10^{16}$ proton/sec,

$\sigma_x = \sigma_y = 1$ mm;

Dump: $\theta_{dump} = 35$ mrad, $S_{ab} \approx \dfrac{2\pi\sigma_x\sigma_y}{\theta_{dump}} \approx 1.8$ cm^2;

Year: $T = 3600\cdot24\cdot365 \approx 3.15\cdot10^7$ sec.

$$V_{atom} = \frac{m_{proton}\cdot M_{atom}}{d};$$

$$S_{[sec]} = Y\cdot N_p, \quad S_{[year]} = S_{[sec]}\cdot T;$$

$$S_{[mm]} = 10\cdot\frac{S_{[year]}\cdot V_{atom}}{S_{ab}}.$$

These input data are used to evaluate the yield for material of PXIE beam dump in continuous operation for one year with 1.7 mA of proton beam with energy 30 MeV.

Value/Material	Nickel	Copper	Carbon	Aluminum	Iron
d, Density, g/cm^3	7.81	8.92	2.267	2.7	7.874
M_{atom}, Weigth of atom, aum	58.69	63.55	12.01	8.27	55.847
V_{atom}, Volume of atom, cm^3	$1.26\cdot10^{-23}$	$1.19\cdot10^{-23}$	$8.9\cdot10^{-24}$	$1.67\cdot10^{-23}$	$1.18\cdot10^{-23}$
Y, Yield, atom/proton	$2.2\cdot10^{-6}$	$4.9\cdot10^{-6}$	$3.4\cdot10^{-7}$	$7.6\cdot10^{-7}$	$1.6\cdot10^{-6}$
$S_{[sec]}$, Sputtering, atom/sec	$2.2\cdot10^{11}$	$4.9\cdot10^{11}$	$3.4\cdot10^{10}$	$7.6\cdot10^{11}$	$1.6\cdot10^{11}$
$S_{[year]}$, Sputtering, atom/year	$6.8\cdot10^{17}$	$1.5\cdot10^{18}$	$1.1\cdot10^{17}$	$2.4\cdot10^{17}$	$5.2\cdot10^{17}$
$S_{[mm]}$, Sputtering, mm/year	$4.8\cdot10^{-5}$	$1.0\cdot10^{-4}$	$5.3\cdot10^{-6}$	$2.2\cdot10^{-5}$	$3.4\cdot10^{-5}$
Maximal values (for corresponding proton energy, keV)					
Y, Yield, atom/proton	$1.7\cdot10^{-2}(\approx 2)$	$3.6\cdot10^{-2}(\approx 2)$	$1.2\cdot10^{-2}(\approx .5)$	$1.8\cdot10^{-2}(\approx .5)$	$1.4\cdot10^{-2}(\approx 2)$
$S_{[sec]}$, Sputtering, atom/sec	$1.7\cdot10^{14}$	$3.6\cdot10^{14}$	$1.2\cdot10^{14}$	$1.8\cdot10^{14}$	$1.4\cdot10^{14}$
$S_{[year]}$, Sputtering, atom/year	$5.2\cdot10^{21}$	$1.1\cdot10^{22}$	$3.7\cdot10^{21}$	$5.6\cdot10^{21}$	$4.4\cdot10^{21}$
$S_{[mm]}$, Sputtering, mm/year	0.367	0.747	0.184	0.524	0.293

These data show that at the current of ~1.7 mA and continuous (during one year), bombarding of nickel beam dump by 30 MeV protons due to sputtering it no more than 0.05 µm of material can be lost due to sputtering. Even at the energy corresponding to the maximum of sputtering yield (~2 keV), the loss will not exceed 0.4 mm per year.

Angular dependence of sputtering yield incident for light ions

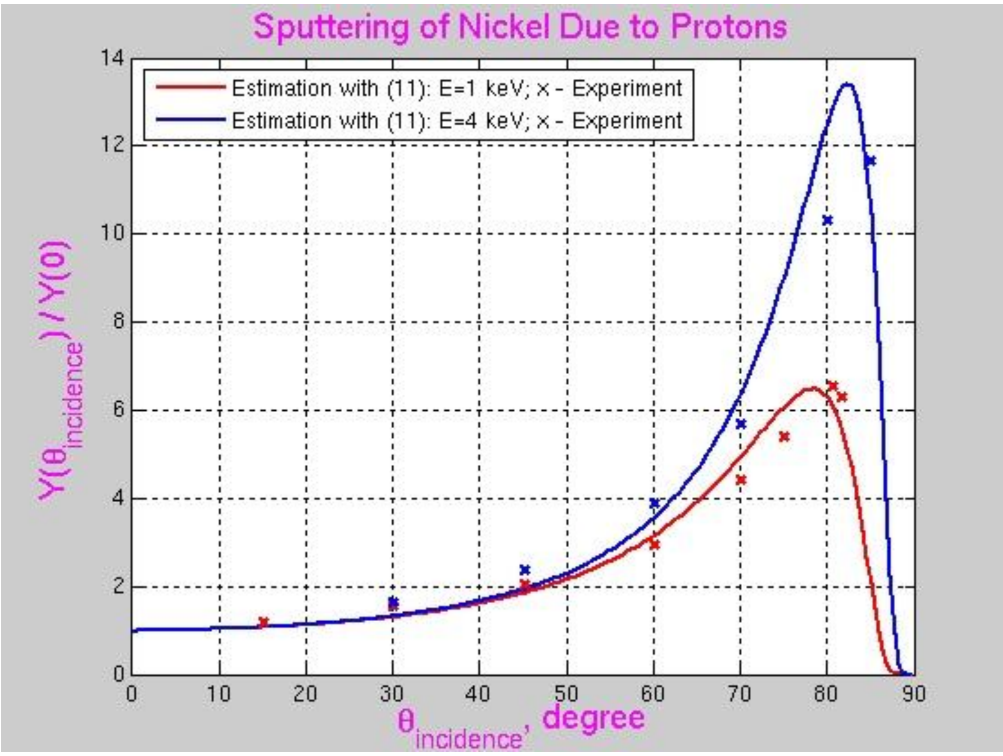
As can be seen from the above table with the data on the possible mechanisms of sputtering at oblique and grazing incidence of light ions to the surface of the target, mechanism I – the direct knock-off of the surface atoms by the incoming incident ions – is predominant. In this case, as shown, both according to the experiments [1, 11, 12] and theoretical analysis [2-4], the yield of sputtered atoms can be much larger than in the case of normal incidence of the beam on the target. For sputtering of light ions the empirical formula, which describes the experimental data well, includes only two fitting parameters f, θ_{opt} and is as follows [13]:

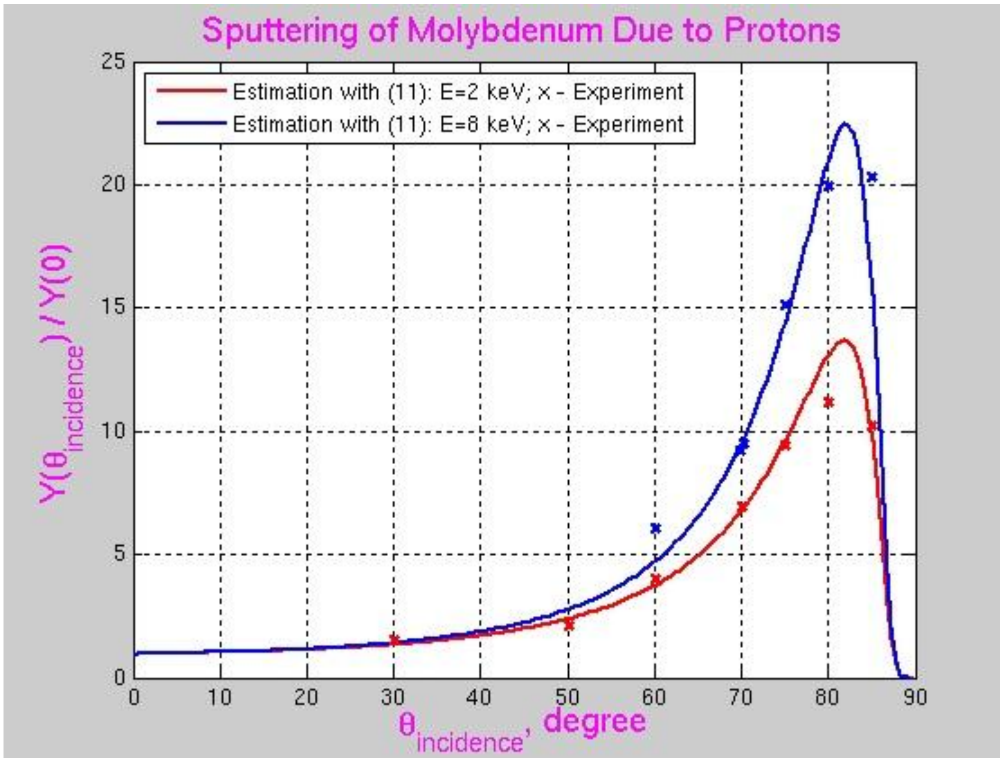
$$Y(\theta) = Y(0)\frac{\exp(-(1/\cos\theta - 1)\cdot\Sigma)}{(\cos\theta)^f}, \text{ where } \Sigma = f\cos\theta_{opt}. \quad (11)$$

These fitting parameters for materials of interest are

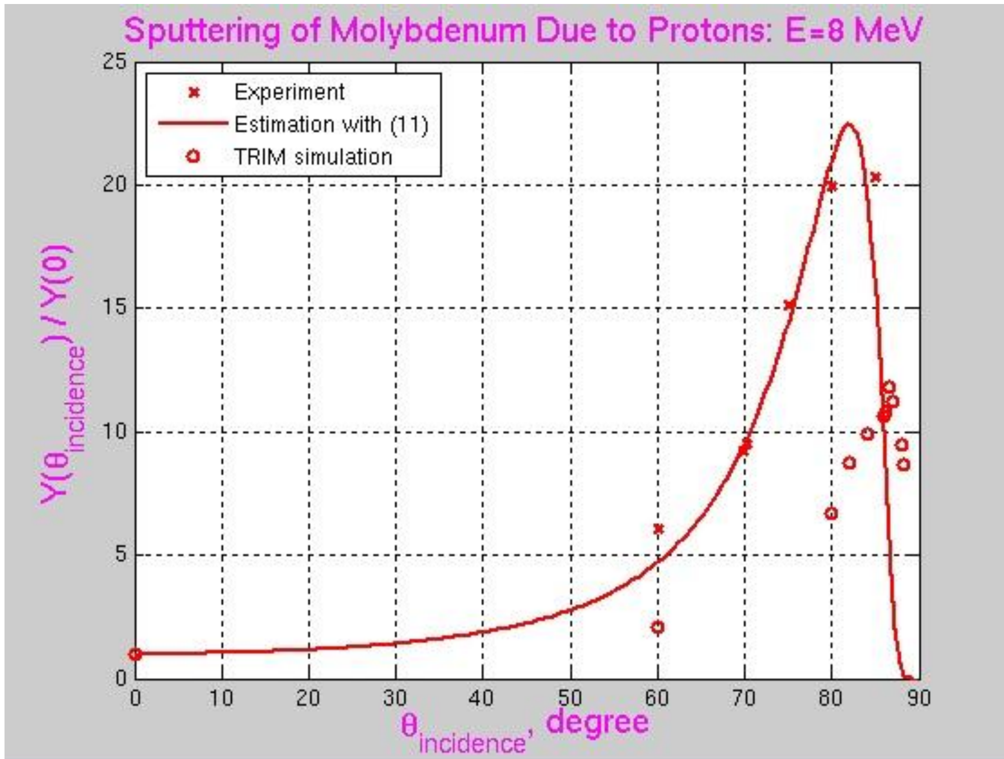
E_{acc}, keV	Target	f	θ_{opt}
2	Mo	2.40	81.8^0
8	Mo	2.80	82.0^0
1	Ni	2.34	78.3^0
4	Ni	2.27	82.3^0

The comparison of experimental data [1] and fitting formula (11) is presented in the following graphs:





As can be seen, the angle with a maximum yield of sputtered atoms increases, as does this yield if the energy of incident beam increases. It means that it is noy possible to use this empirical expression for the energies of the order of 2.1 MeV (MEBT absorber) and even more so for the 30 MeV (PXIE beam dump). Therefore, code TRIM was used for the desired estimates. Previously this program was used to calculate the angular distribution of sputtered atoms yield for the molybdenum target and incident proton beam with the energy of 8 keV. It allowed comparing the result with the experimental data and empirical evaluation by the formula (11). It should be taken into account that the statistical accuracy of the TRIM calculations for parameters under consideration is low (approximately 50%). The results are presented in the following graph:



Unfortunately, it is clear that for some reason the version of TRIM used in this case produces the result different from the experimental data almost twofold and also the angle corresponding to the maximum yield is very different too. Generally speaking, there is a special version of the code TRIM: TRIM.SP [14, 15] created specifically to simulate the sputtering process. This version besides the Monte Carlo approach contains an additional block to calculate the collisions of the particles (of the initial beam and the atoms of the medium) in BCA approximation. However, unfortunately, it remains unknown exactly which version of TRIM was used in the cited calculations of the sputtering. Thus, we cannot use the code TRIM for the numerical estimates of the number of sputtered atoms in the cases of MEBT absorber and PXIE beam dump.

Conclusions

It is shown that the parameters of the proton beam in the fall it on molybdenum MEBT absorber (2.1 MeV x 10 mA = 21 kW) and on the nickel PXIE beam dump (30 MeV x 1.7 mA = 50 kW) the phenomenon of sputtering target material is negligible in terms of expected duration of operation of these devices.

References

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